

Resonance Region Quality Assurance

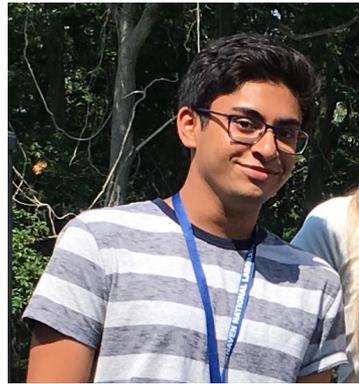
David Brown

NNDC, Brookhaven National Laboratory

BROOKHAVEN
NATIONAL LABORATORY

 U.S. DEPARTMENT OF
ENERGY

My collaborators on this project



Rishi Wadgoankar
(HSRP student)



Declan Mulhall
(Univ. Scranton)

ADVANCE continuous integration system key for ENDF QA

- Check new evaluations every commit
- Uses customer codes (NJOY, FUDGE, PREPRO)
- Automates ENDF Phase I testing
- Build reports for variety of needs



In process of upgrading backend to Python3, BuildBot 2.10 on new server

The screenshot displays the BuildBot web interface in a Mozilla Firefox browser window. The address bar shows the URL `localhost:10005/#/builders/2/builds/1`. The interface includes a left-hand navigation menu with options like Home, Grid View, Waterfall View, Console View, Builds, Builders, Pending Buildrequests, Last Changes, Build Masters, Schedulers, Workers, About, and Settings. The main content area shows the details for build `build-alphas / 1`, which is marked as "Finished a few seconds ago". Below this, there are tabs for "Build steps", "Build Properties", "Worker: workerCP", "Responsible Users", "Changes", and "Debug". The "Build steps" tab is active, showing a list of steps: "All build-alphas/1 | force build" (failed), "svn" (1 s update), and "shell" (failed). A "studio" view is expanded, showing a terminal window with the following environment variables:

```
40 PSTLR00T=/opt/intel/compilers_and_libraries_2018.2.199/linux/pstl
41 PWD=/home/dbrown/advance.trunk/work/endif/workerCP/build-alphas/build
42 PYTHONPATH=/home/dbrown/fudge.trunk:/home/dbrown/advance.trunk:/home/dbrown/x41.trunk:.
43 QTDIR=/usr/lib64/qt-3.3
44 QTINC=/usr/lib64/qt-3.3/include
45 QTLIB=/usr/lib64/qt-3.3/lib
46 QT_GRAPHICSSYSTEM_CHECKED=1
47 QT_PLUGIN_PATH=/usr/lib64/kde4/plugins:/usr/lib/kde4/plugins
48 SELINUX_LEVEL_REQUESTED=
49 SELINUX_ROLE_REQUESTED=
50 SELINUX_USE_CURRENT_RANGE=
51 SHELL=/bin/bash
52 SHLVL=2
53 SSH_CLIENT=130.199.210.237 55869 22
54 SSH_CONNECTION=130.199.210.237 55869 130.199.66.202 22
55 SSH_TTY=/dev/pts/0
```

The bottom left corner features the U.S. Department of Energy logo, and the bottom right corner features the IEN ATORY logo.

In process of upgrading backend to Python3, BuildBot 2.10 on new server

Buildbot Builders / build-alphas / 1

Rebuild

Finished a few seconds ago

Developing resonance quality report

instance.py -c ...' (failure) **FAILURE**

1 s update

'setup_ci_instance.py -c ...' (failure)

stdio view all 80 lines download

```
40 PSTLR00T=/opt/intel/compilers_and_libraries_2018.2.199/linux/pstl
41 PWD=/home/dbrown/advance.trunk/work/endif/workerCP/build-alphas/build
42 PYTHONPATH=/home/dbrown/fudge.trunk:/home/dbrown/advance.trunk:/home/dbrown/x41.trunk:.
43 QTDIR=/usr/lib64/qt-3.3
44 QTINC=/usr/lib64/qt-3.3/include
45 QTLIB=/usr/lib64/qt-3.3/lib
46 QT_GRAPHICSSYSTEM_CHECKED=1
47 QT_PLUGIN_PATH=/usr/lib64/kde4/plugins:/usr/lib/kde4/plugins
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```

What kinds of things get us into trouble in the resonance region?

What kinds of things get us into trouble in the resonance region?

- Missing resonances
- Miss-assigned resonances

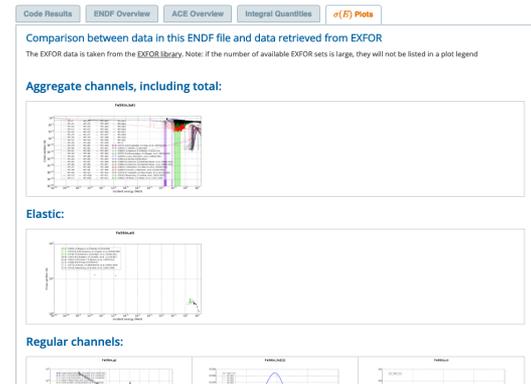
Focus of this work

What kinds of things get us into trouble in the resonance region?

- Missing resonances
- Miss-assigned resonances
- Missing or incorrect backgrounds
- Bad fits to experiment

Focus of this work

Visual inspection of plots



What kinds of things get us into trouble in the resonance region?

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- Missing channels

Focus of this work

Visual inspection of plots

FUDGE & PREPRO check

The screenshot displays the 'Code Results' tab of the ADVANCE Continuous Integration System. It features a table summarizing tests on the evaluation. The table has columns for Code, Status, Code, # Tests, # Failures, # Errors, Run time, and Files. The tests listed are STAN, STANEP, CHECKA, FUDGE, PSYCHE, INTER, LINEAR, and SIGMA. The FUDGE test is highlighted in red, indicating a failure.

Code	Status	Code	# Tests	# Failures	# Errors	Run time	Files
ENDF		STAN	0	0	0	0.831	
NUDC Codes		STANEP	0	0	0	0.837	
		CHECKA	57	0	0	0.203	
		FUDGE	56	1	1	38.223	LOG
		PSYCHE	96	0	0	0.198	
		INTER	1	0	0	0.062	inter_file
PREPRO		LINEAR	67	0	0	0.221	linear_file
		SIGMA	69	0	0	42.746	sigma_file

What kinds of things get us into trouble in the resonance region?

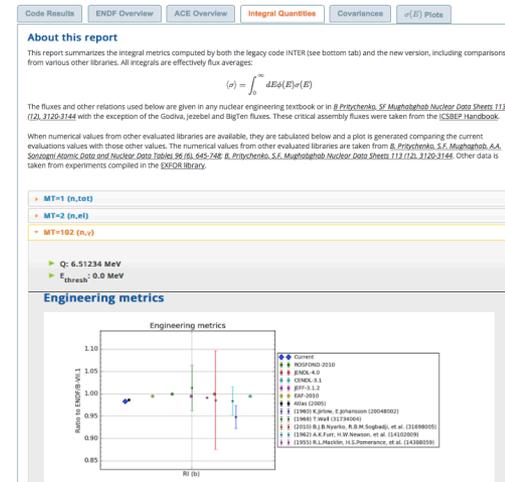
- Missing resonances
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- Bad fits to experiment
- Missing channels
- Bad match to integral quantities (RI, thermal cross section, MACS, Westcott factor, ...)

Focus of this work

Visual inspection of plots

FUDGE & PREPRO check

ADVANCE's integral metric report covers this



What kinds of things get us into trouble in the resonance region?

- Missing resonances
- Miss-assigned resonances
- Missing or incorrect backgrounds
- Bad fits to experiment
- Missing channels
- Bad match to integral quantities (RI, thermal cross section, MACS, Westcott factor, ...)
- Inconsistent with the Atlas
- RRR-URR inconsistency

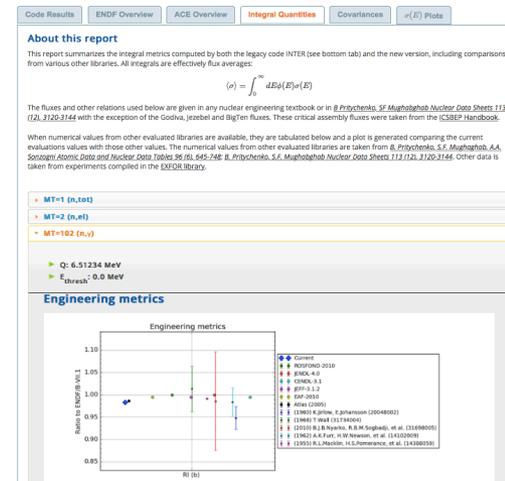
Working on it!

Focus of this work

Visual inspection of plots

FUDGE & PREPRO check

ADVANCE's integral metric report covers this



Resonance metrics to consider

Measures of energies

- **Long range behavior**
 - Average spacing vs. E
 - Cumulative level distribution
- **Short range behavior**
 - Nearest neighbor spacing distribution
 - Spacing-spacing correlation
 - Dyson-Mehta Δ_3 statistic
 - Other statistics

Measures of widths

- **Long range behavior**
 - Average width vs. E
 - Width distribution
- **Short range behavior**
 - Are there short range correlations in the widths?

Resonance metrics to consider

Measures of energies

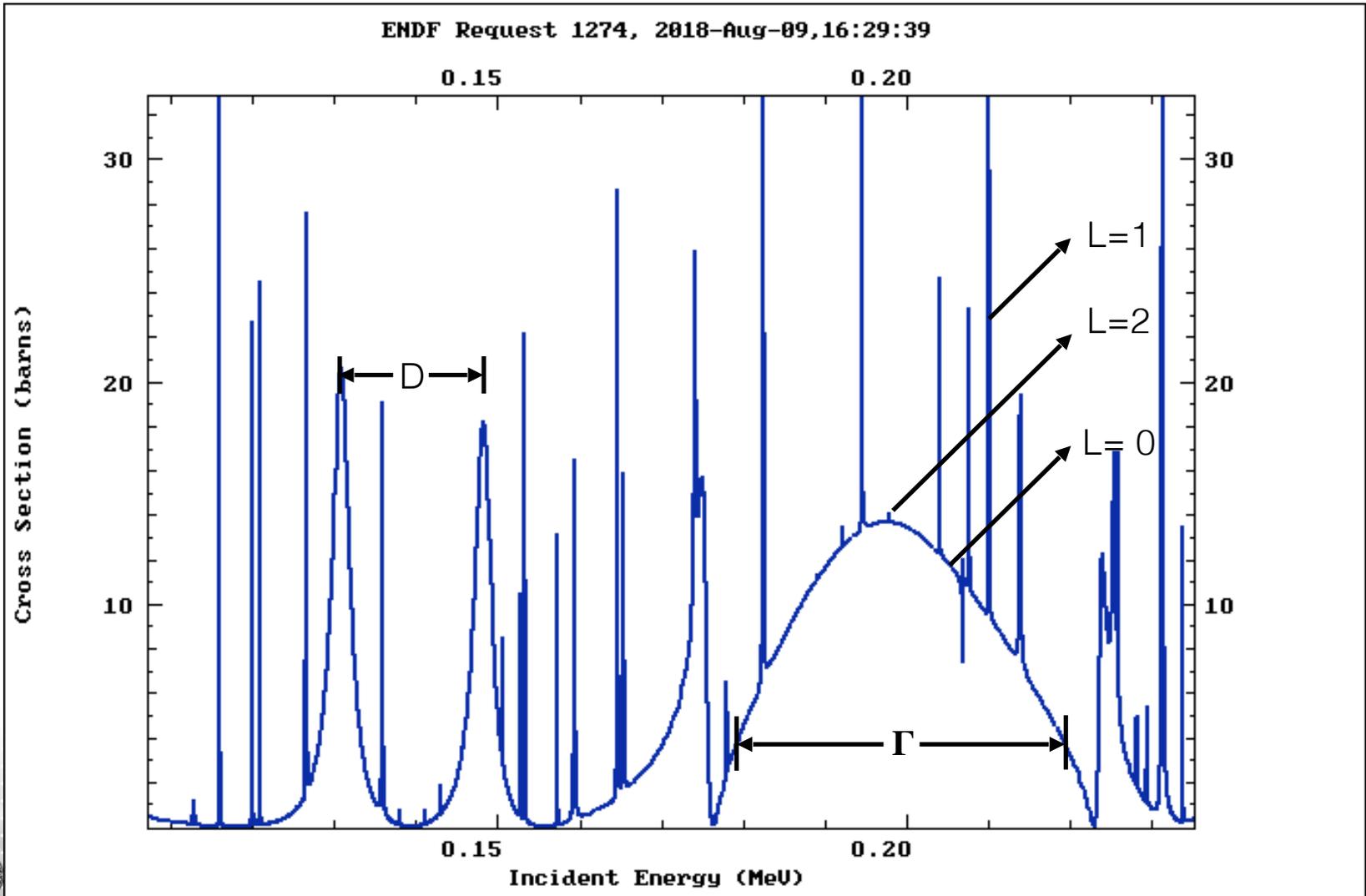
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In most cases, have analytic results from random matrix theory as guide

Typical resonance region



Resonance metrics to consider

Measures of energies

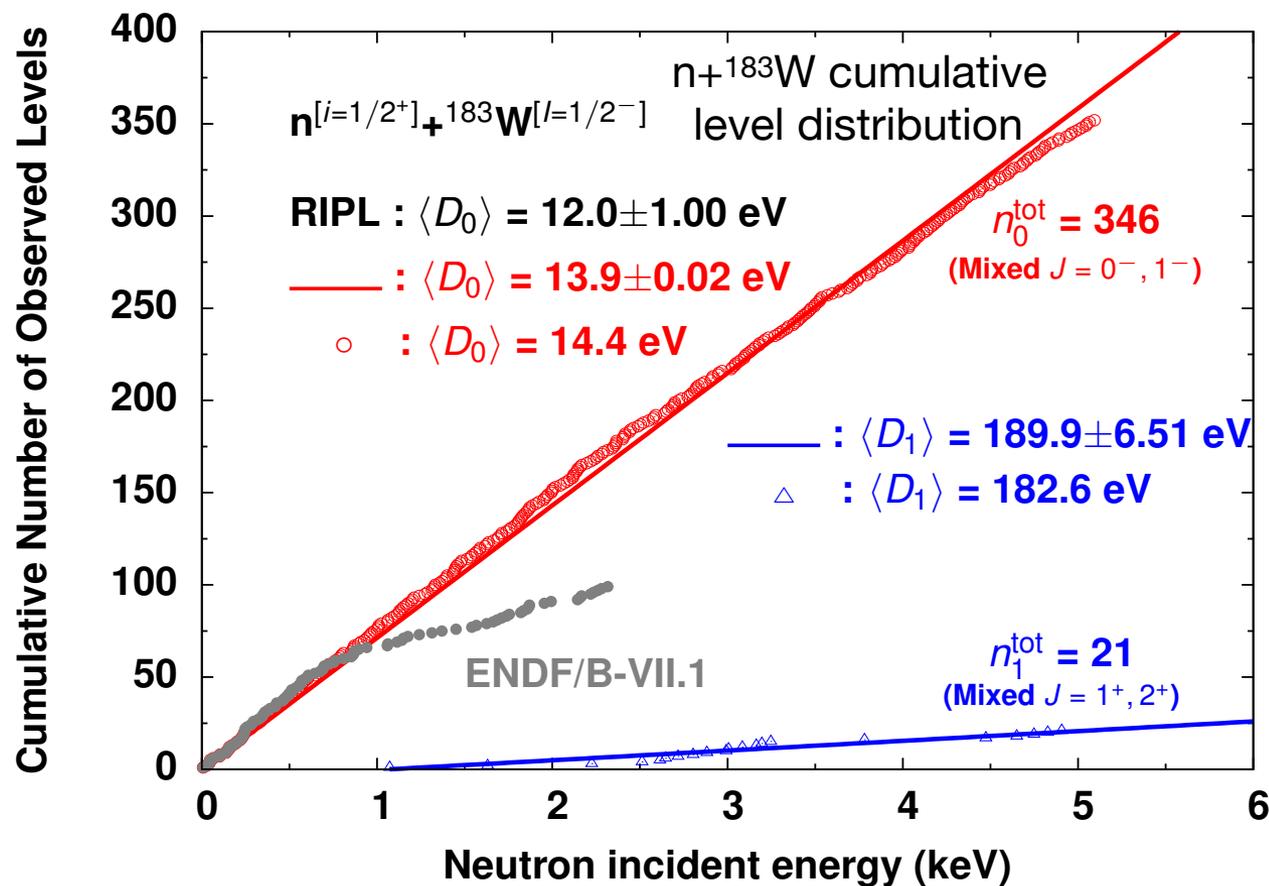
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Measures of widths

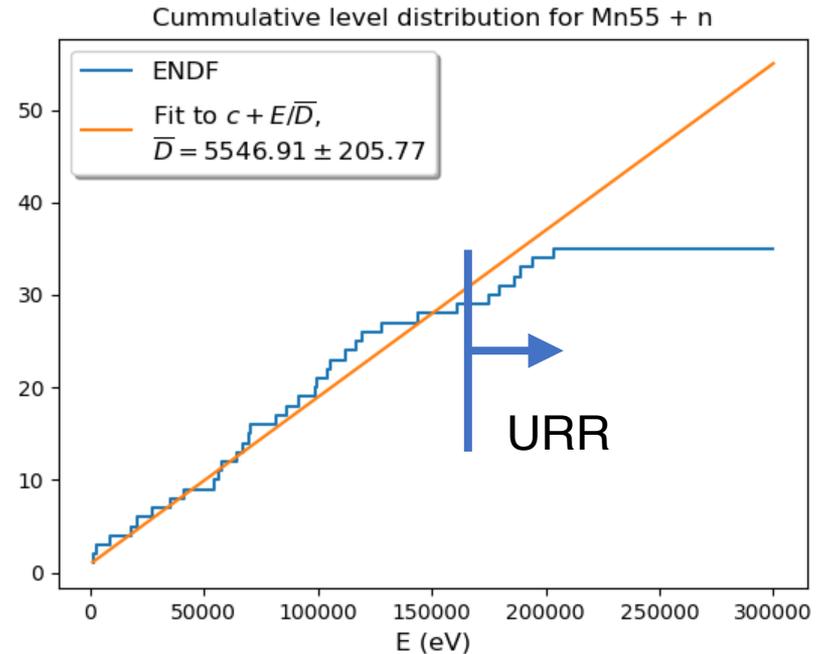
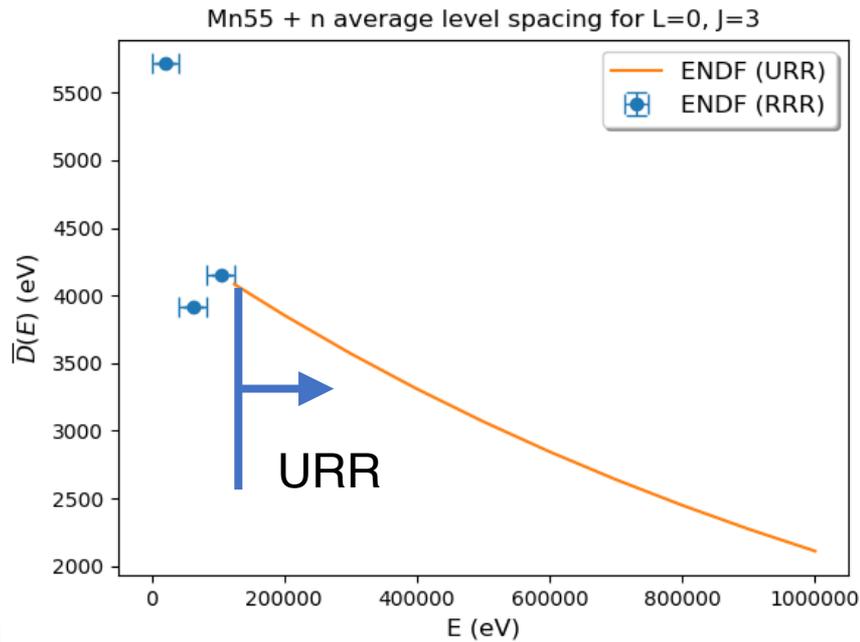
- Long range behavior
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Cumulative level distribution already tells us a lot

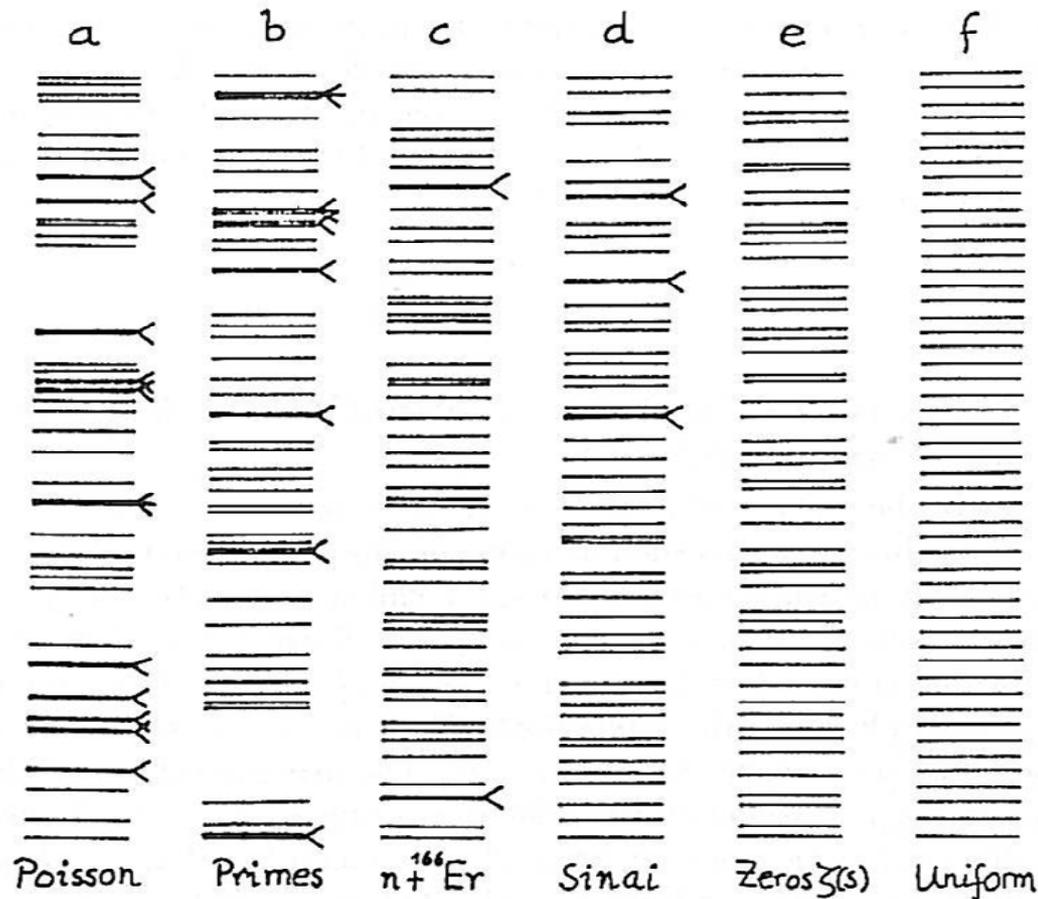
- Is the average spacing correct?
- Missing levels manifest as deviations from straight line



Application to ^{55}Mn shows good RRR-URR transition; before missing lots of levels

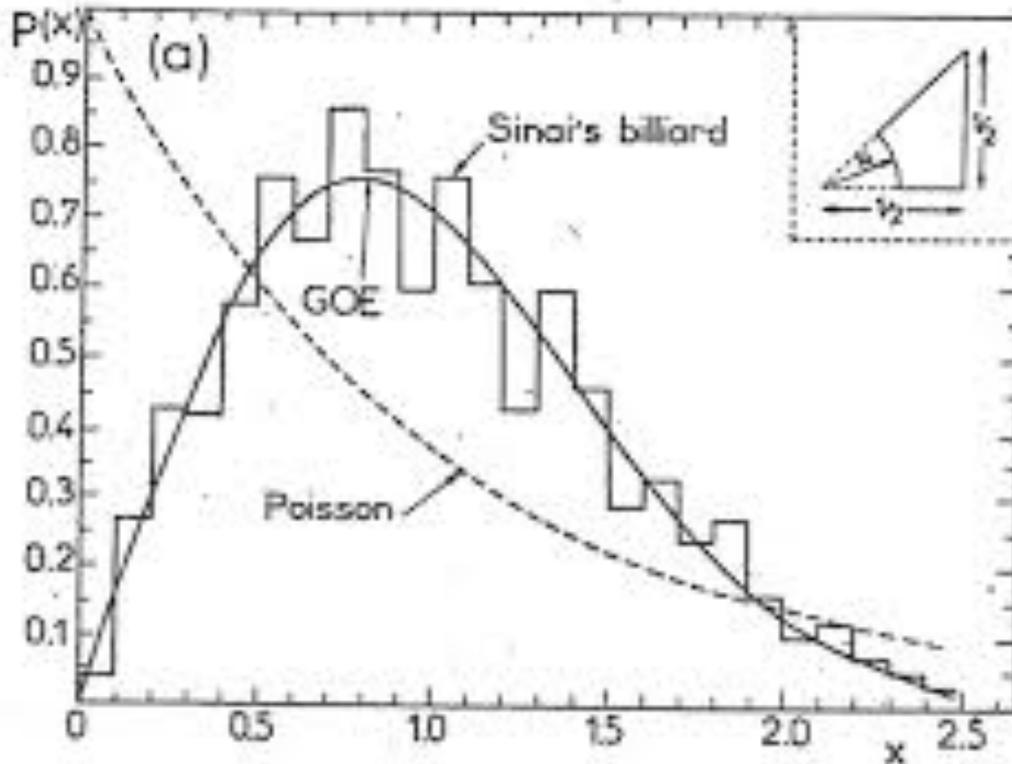


Look at resonance spacings



O. Bohigas and M. J. Giannoni, Lecture Notes in Physics 209 (1984), Springer-Verlag, Heidelberg

Nearest neighbor spacing distribution



Nearest neighbor spacing is simply

$$D_i = E_{i+1} - E_i$$

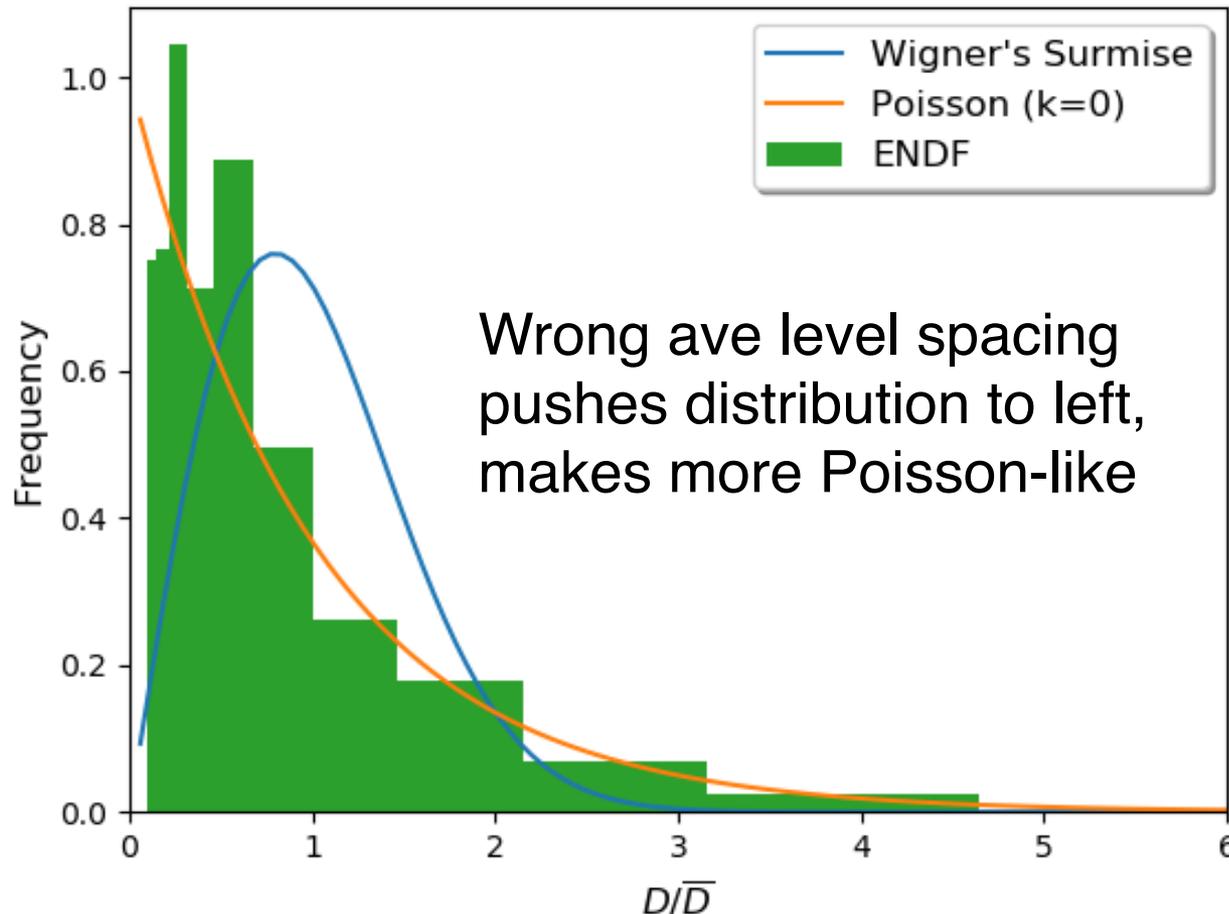
So, make a histogram with

$$x = D_i / D$$

Bohigas, Giannoni, Schmitt, Phys. Rev. Lett. **52**, p. 1 (1984)

Can immediately tell that levels are missing based on shape or shift in x-axis scaling

K41 + n nearest neighbor spacing distribution for L=1, J=3



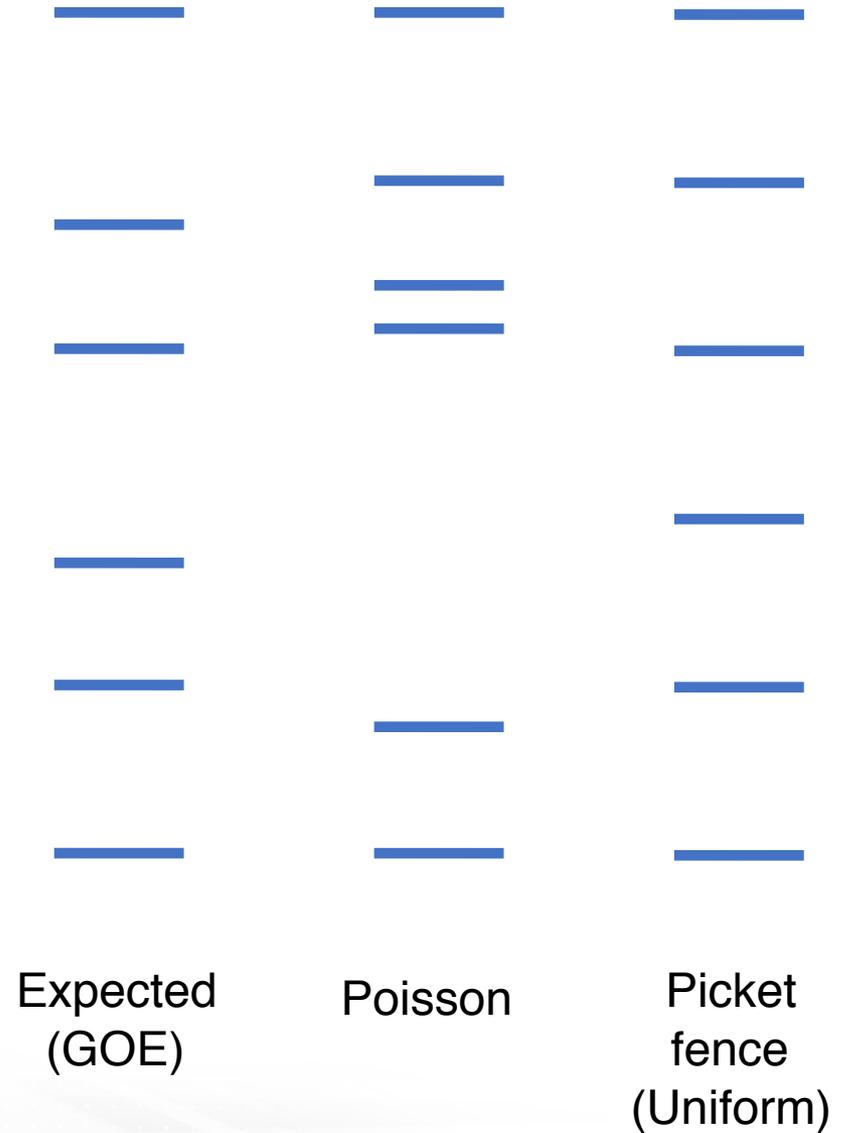
$$P_{GOE}(x) = \frac{\pi}{2} x e^{-\pi x^2/4}$$

vs.

$$P_P(x) = \frac{x^k e^{-x}}{k!}$$

Spacings tell us a lot more

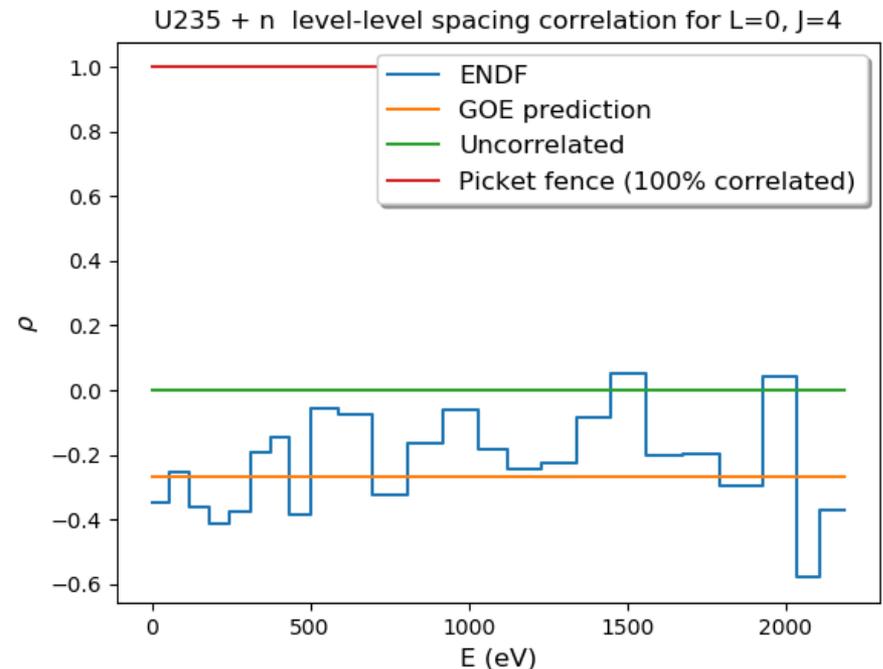
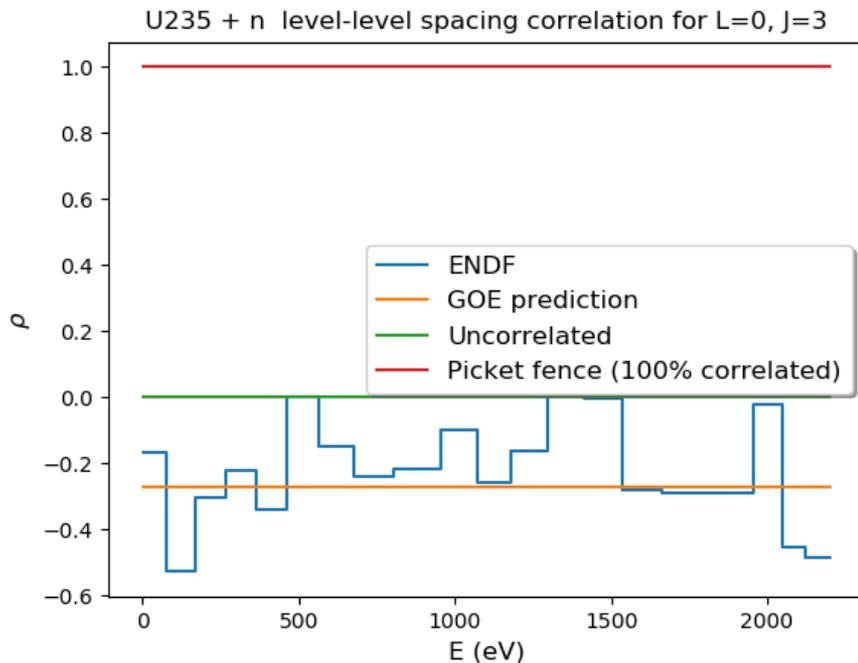
- Poisson too random: has big gaps and big clusters
- Picket fence too regular
- GOE just right
 - S-L-S-L spacing correlation
 - Almost as regular as picket fence



ρ , the spacing-spacing correlation

$$\begin{aligned}\rho(D_i, D_{i+1}) &= \text{corr}(D_i, D_{i+1}) \\ &= \frac{\sum_i (D_i - \bar{D})(D_{i+1} - \bar{D})}{\sum_i (D_i - \bar{D})^2}\end{aligned}$$

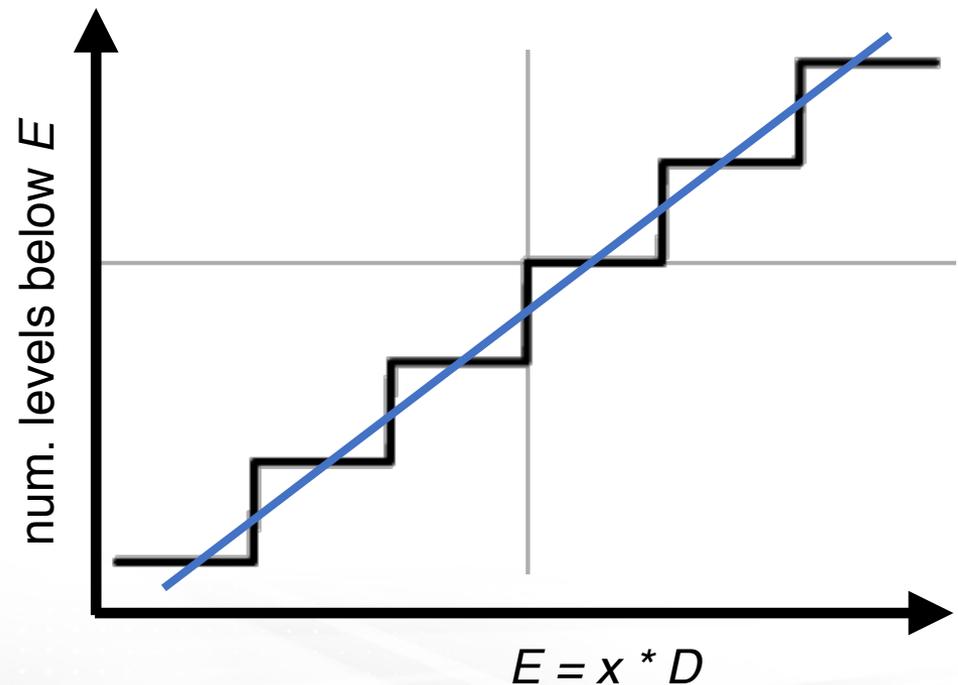
S-L-S-L pattern gives correlation coefficient of -0.27 for GOE



Dyson-Mehta Δ_3 statistic

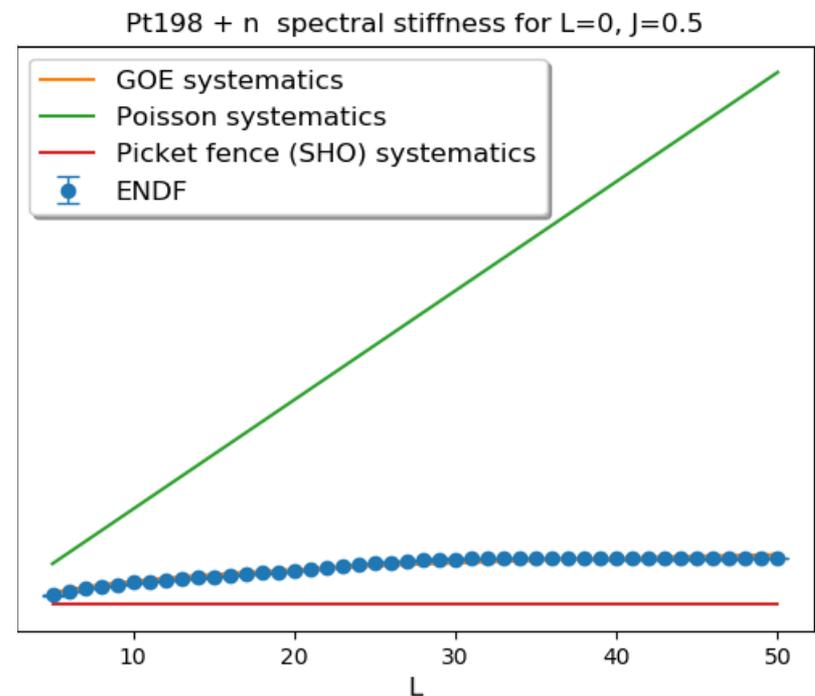
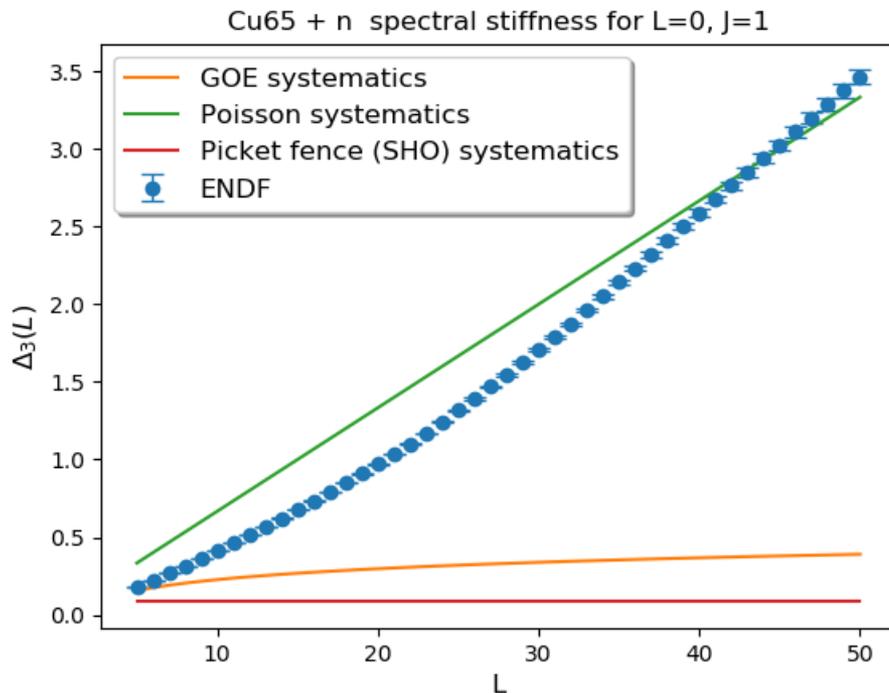
- A fancy sounding name
- Measures “spectral stiffness”
- Really just based on straight line fit to cumulative level distribution
- Vary number of steps (L) used in fit
- Know expected slope as function of L

$$\Delta_3(r) = \frac{d}{2L} \min_{A,B} \int_{x-L}^{x+L} [F(x') - Ax' - B]^2 dx'$$



Dyson-Mehta Δ_3 statistic

- Know expected values of Δ_3 for picket fence (regular), GOE (realistic) and Poisson (random)
- ^{65}Cu indicates significant admixture of resonances from other channel
- ^{198}Pt does NOT indicate complete set of resonances, rather indicates quality of fake resonances generated by TARES



Other metrics

- U statistic “thermodynamic energy”
 - Q statistic
 - F statistic
 - ...
-
- All give essentially same information as Δ_3

Resonance metrics to consider

Measures of energies

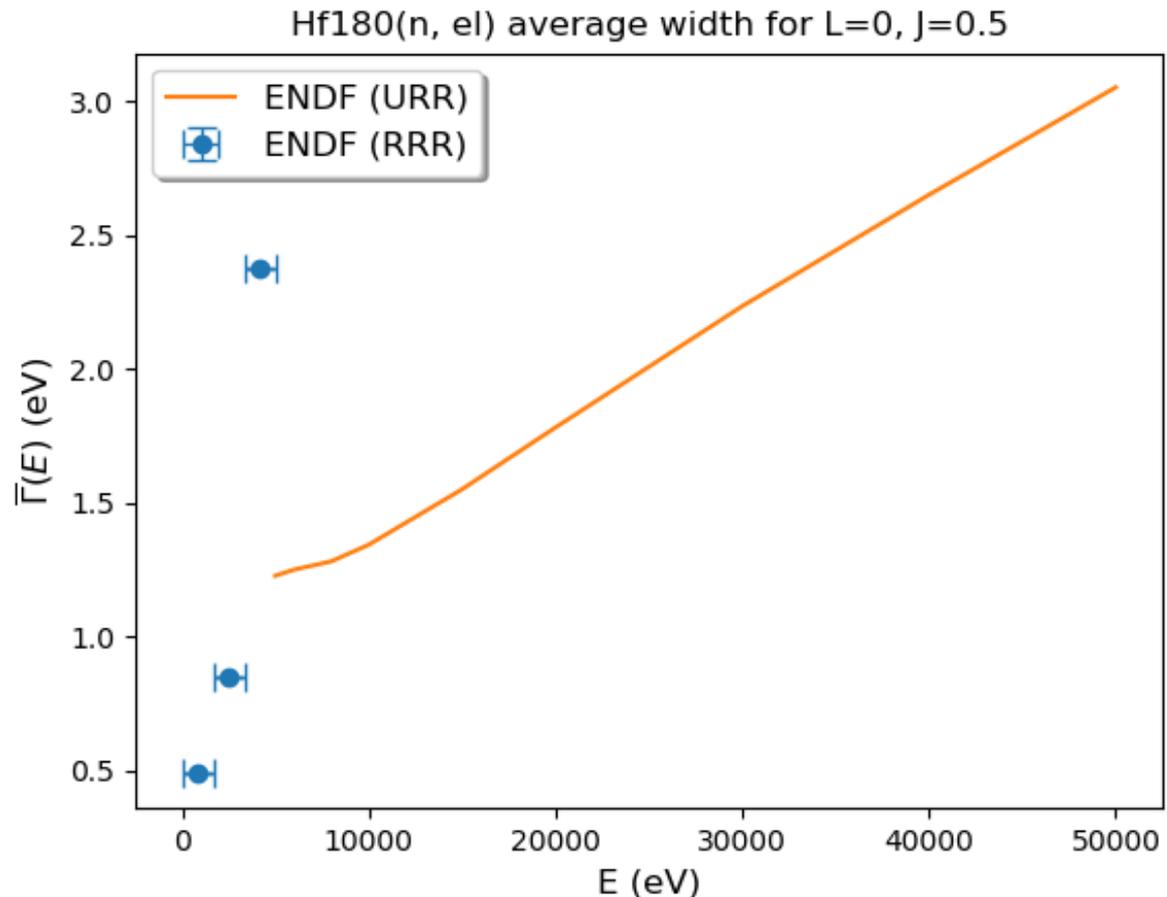
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Measures of widths

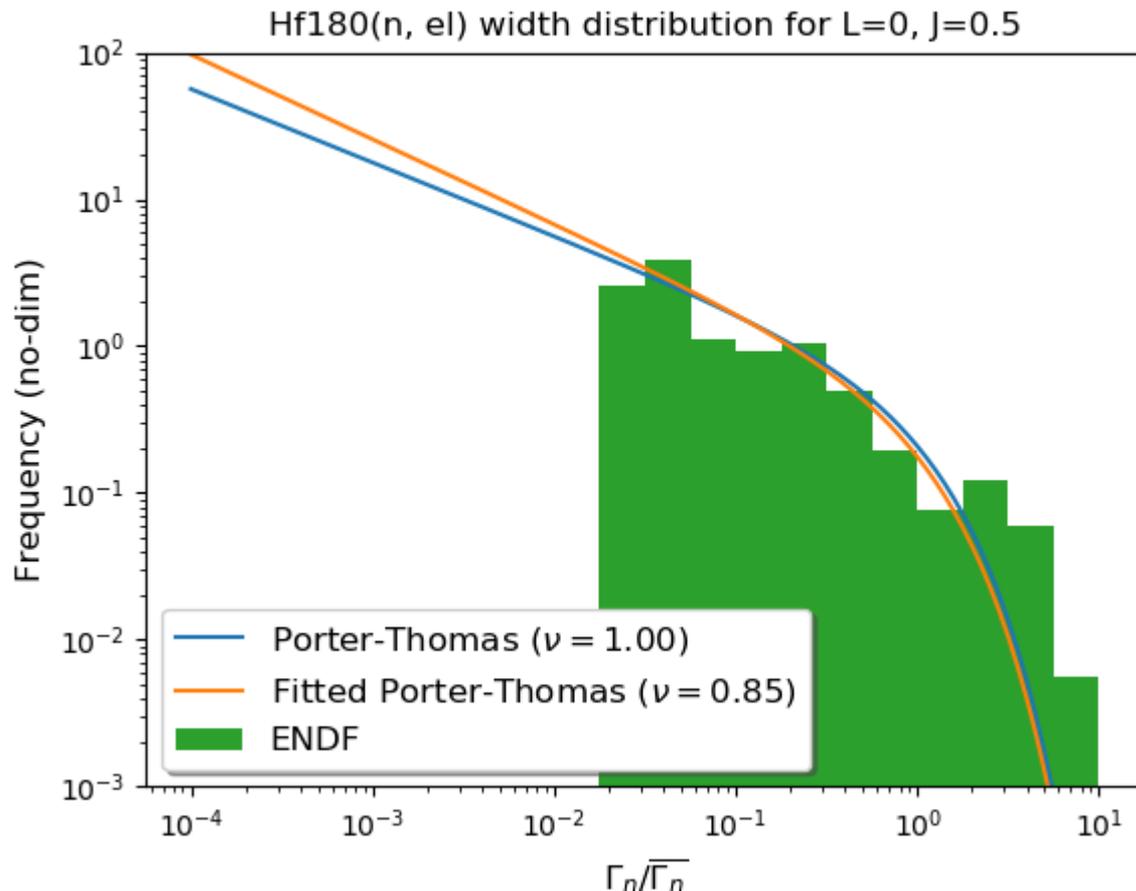
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Plot average with to show consistency between RRR & URR

- Gamma widths usually small, not vary much
- Neutron widths, must be careful about “reduced width” in URR

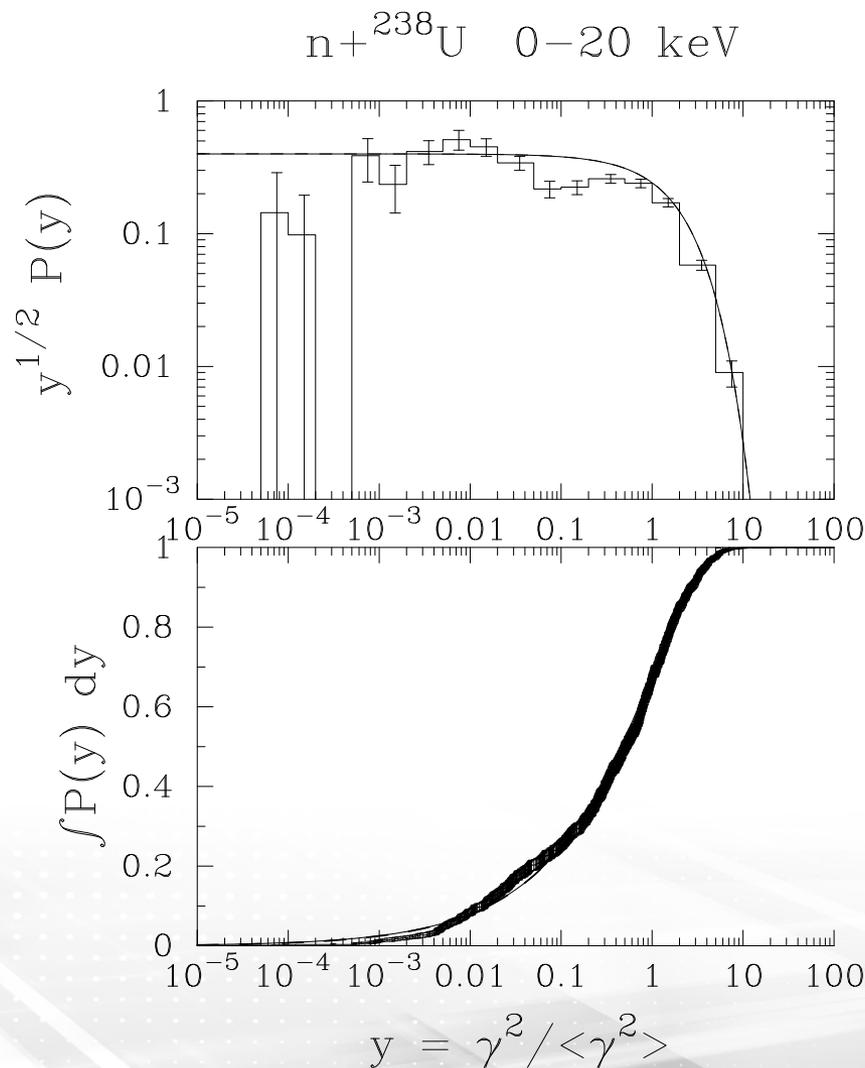


Width distribution commonly used to assess for missing levels



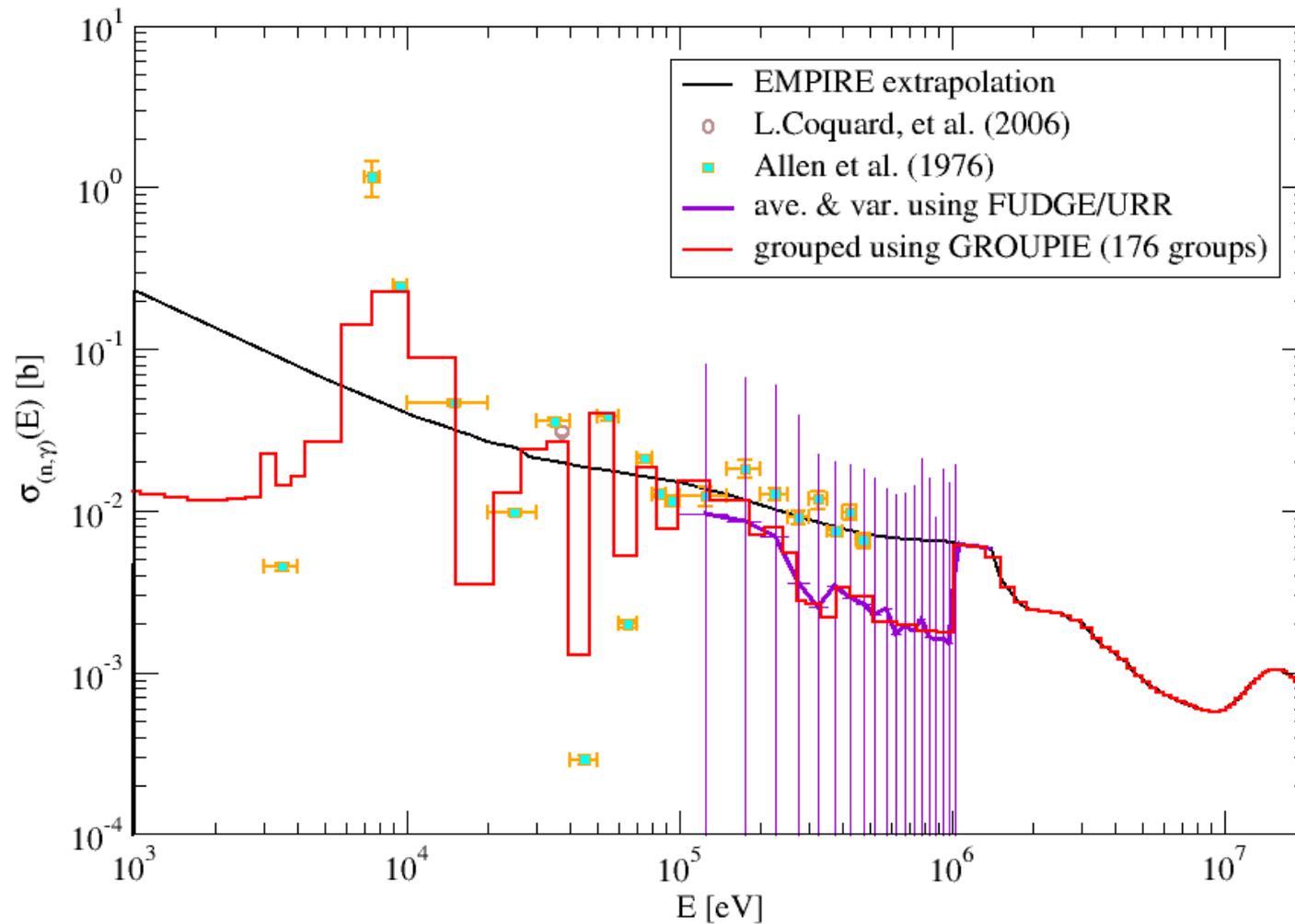
- A lot of literature using this to assess missing levels
- Wrong ave width pushes distribution to left
- Missing levels have small width

Other ways of displaying width distribution are more informative, must investigate



Mitchel, Shriner,
NDC(NDS)-0561
(2009)

^{54}Fe capture: group averaged capture resonances reveals missing strength from 200 keV - 1 MeV, likely from missing p-, d- wave resonances



Mitchell and Shriner missing level study INDC(NDS)-0561



IAEA
International Atomic Energy Agency

INDC(NDS)-0561
Distr. G+NM

INDC International Nuclear Data Committee

Missing Level Corrections using Neutron Spacings

G.E. Mitchell

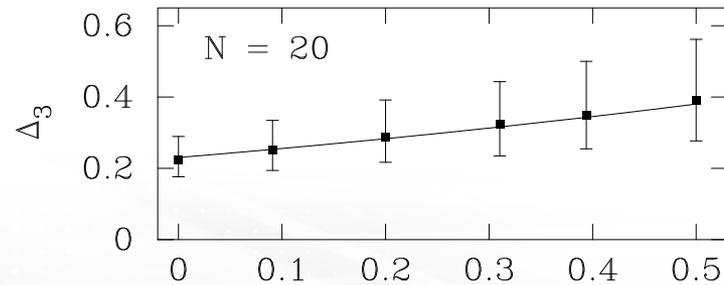
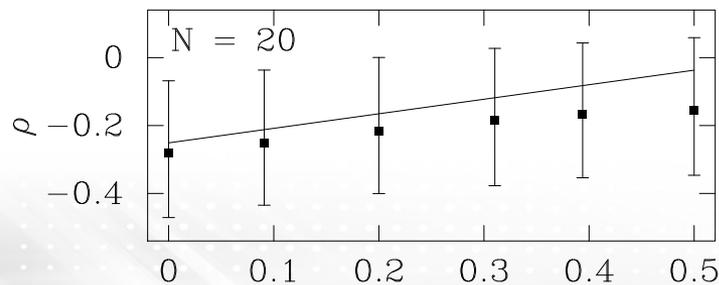
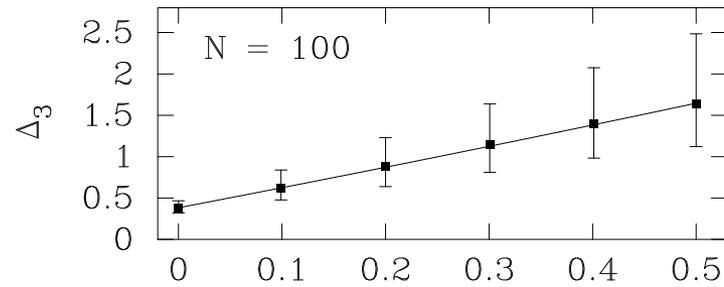
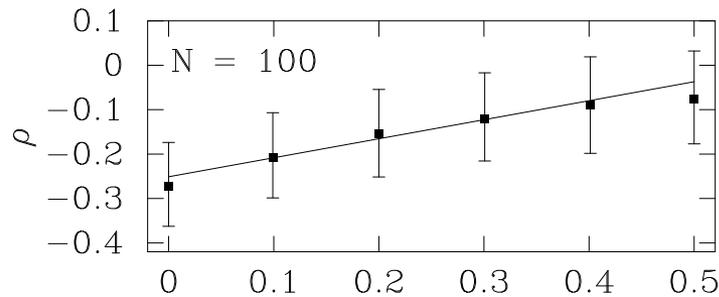
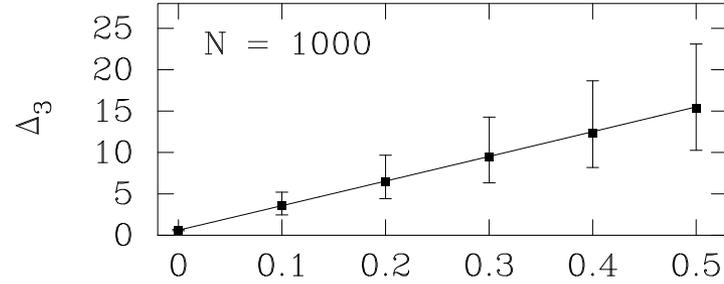
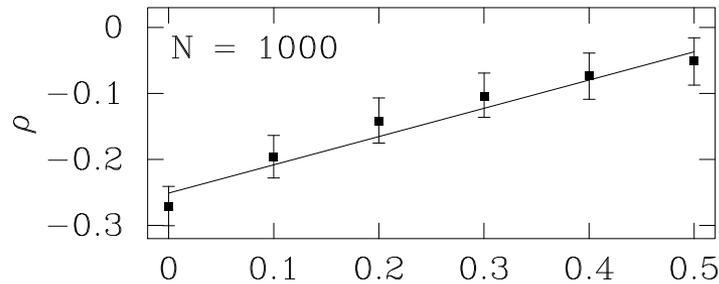
North Carolina State University and
Triangle Universities Nuclear Laboratory

and

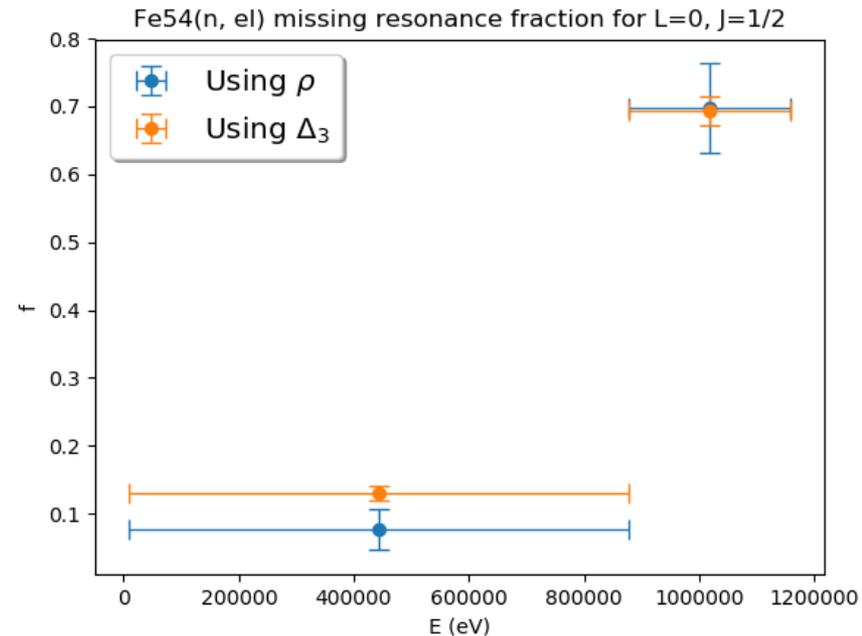
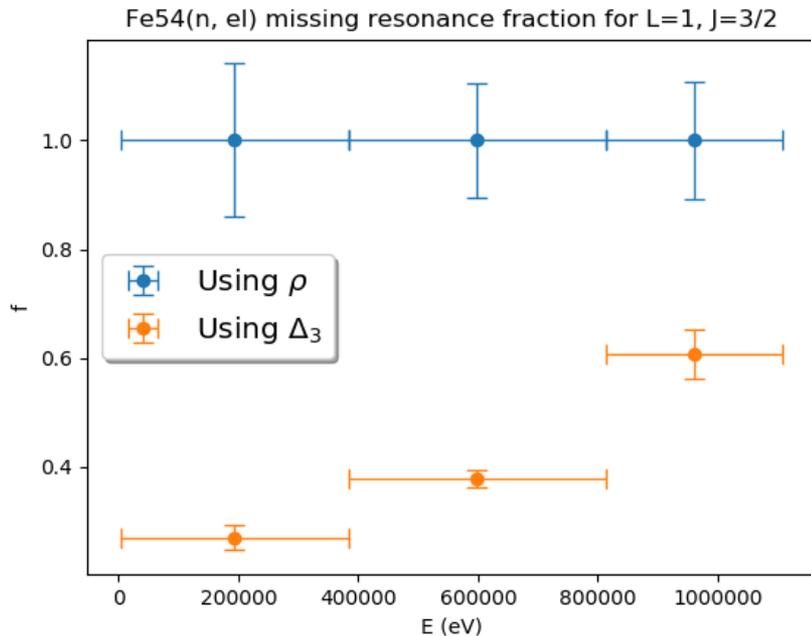
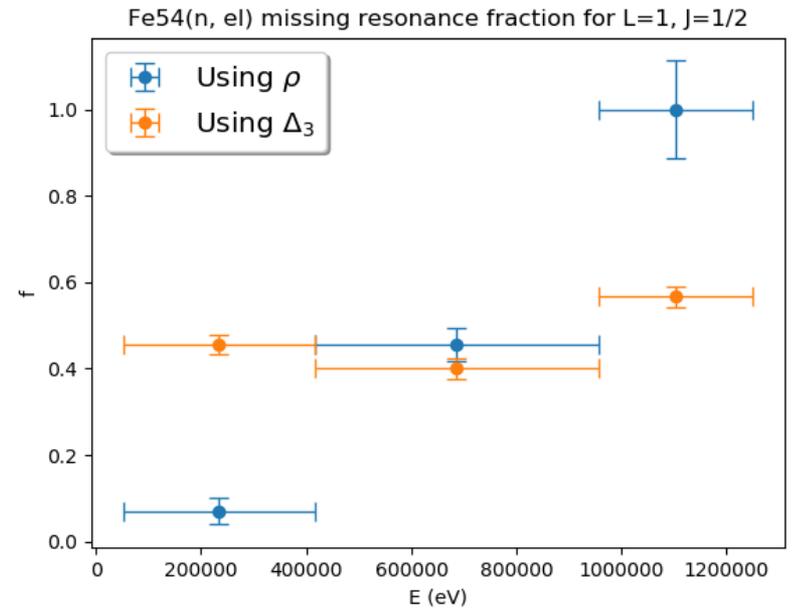
J.F. Shriner, Jr.

Tennessee Technological University

Systematics of ρ & Δ_3 as function of # levels & fraction missing



Can we use these to assess the fraction of missing resonances?



Status

- Lab report detailing system available (BNL-209313-2018-INRE)
- Aiming for rollout of report before next CSEWG
- Investigating combining width & Dyson-Mehta metrics for more holistic estimate of missing/miss assigned levels
- Investigating RRR-URR constancy approaches

Brookhaven National Laboratory Report
BNL-209313-2018-INRE

A tale of two tools: `mcres.py`, a stochastic resonance generator, and `grokres.py`, a resonance quality assurance tool

David Brown,^{1,*} Declan Mulhall,^{2,†} and Rishi Wadgoankar³

¹*National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY*

²*University of Scranton, Scranton, PA*

³*G.W. Hewlett High School*

(Dated: October 19, 2018)

We detail two software tools, now integrated into the `fudge` code system. The first tool, `mcres.py`, can be used to generate stochastic ensembles of resonances which are both consistent with the expectations of the Gaussian Orthogonal Ensemble of Random Matrix Theory and with the level densities and widths encoded in ENDF formatted files. The second tool, `grokres.py`, can be used to